

Product Name: ATC 0065

Catalog No.: 3359

Batch No.: 1

CAS Number: 510732-84-0

IUPAC Name: *N*²-[*cis*-4-[[2-[4-Bromo-2-(trifluoromethoxy)phenyl]ethyl]amino]cyclohexyl]-*N*⁴,*N*⁴-dimethyl-2,4-quinazolinediamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₉BrF₃N₅O.2HCl.½H₂O

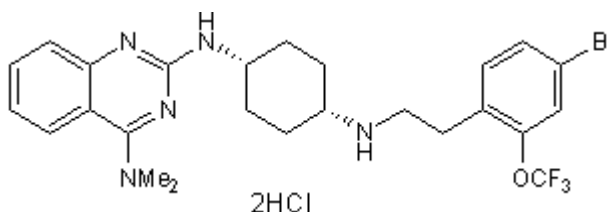
Batch Molecular Weight: 634.36

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 47.33 | 5.08 | 11.04 |
| Found | 47.27 | 5.12 | 10.89 |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Orally active, potent and selective melanin-concentrating hormone receptor 1 (MCH₁) antagonist (IC₅₀ = 15.7 nM) that displays > 96-fold selectivity over MCH₂. Exhibits antidepressant and anxiolytic activity in vivo. Also displays affinity for 5-HT_{1A} and 5-HT_{2B} receptors (IC₅₀ values are 62.9 and 266 nM respectively).

Physical and Chemical Properties:

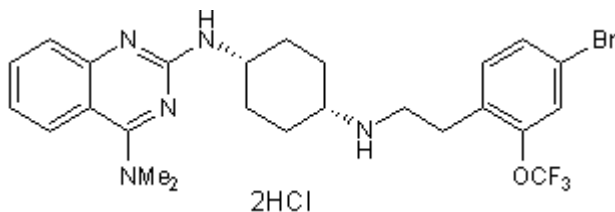
Batch Molecular Formula: C₂₅H₂₉BrF₃N₅O.2HCl.½H₂O

Batch Molecular Weight: 634.36

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Chaki et al (2005) Anxiolytic- and antidepressant-like profile of ATC0065 and ATC0175: Nonpeptide and orally active melanin-concentrating hormone receptor 1 antagonists. *J.Pharmacol.Exp.Ther.* **313** 832.

Dyck et al (2005) Small molecule melanin-concentrating hormone receptor 1 (MCH1R) antagonists as anxiolytic and antidepressive agents. *Drug Dev.Res.* **65** 291.

Kanuma et al (2006) Identification of 4-amino-2-cyclohexylaminoquinazolines as metabolically stable melanin-concentrating hormone receptor 1 antagonists. *Bioorg.Med.Chem.* **14** 3307. PMID: 16434202.

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